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Statistical thermodynamic approach to molten Fe–Cr–P

Statistical thermodynamic analysis was applied to the available phosphorus solubility data set for molten $Fe_{1-y}Cr_yP_x$ given as functions of Cr composition y, temperature T and phosphorus activity $a(P)$ under the assumption that the solubility limit x of P in the molten $Fe_{1-y}Cr_y$ was 0.50 irrespective of y. The evaluated values of the energy parameter representing the extent of stability of P atoms in the molten $Fe_{1-y}Cr_yP_x$ showed an apparently realistic variation pattern with y for the level of y up to 0.465. Further, it was demonstrated by an interpolating estimation using the obtained statistical thermodynamic parameter values at two known levels of y that $a(P)$ vs. x relationships for arbitrary y at specified T could be derived with acceptable accuracy.

Keywords: Molten Fe–Cr–P; Non-stoichiometry; Interstitial compound; Phosphorus activity; Statistical thermodynamics

1. Introduction

Equilibrium $a(P)-T-C$ (phosphorus activity–temperature–composition) relationships for the molten Fe–Cr–P system were determined by Zaitsev et al. [1] using the Knudsen effusion technique over molten $Fe_{1-y}Cr_yP_x$ for sets of fixed compositions, x and y, by varying temperature T in the range between 1820 K and 1400 K over the range of y between 0.06 and 0.93 and x up to 0.47. The reported discrete set of $a(P)-T-C$ relationships were consisted of totally 84 data points (see Table 1 in Ref. [1] for original data set or Table 1 in Ref. [2] with a converted composition expression in $Fe_{1-y}Cr_yP_x$ format). Note that x_P for the experimental runs 73 ~ 76 in Table 1 of Ref. [2] was mis-typed to be 0.146 in place of the correct 0.143. Such discrete $a(P)-T-C$ data presentation was not very convenient for further thermodynamic or statistical thermodynamic analysis and thence an attempt was made to derive an empirical analytical expression for composition x for given y as functions of T and $a(P)$ in a standardised analytical form [2]

$$x = A \cdot a(P) \cdot \exp(B \cdot \ln T + C/T) \qquad (1)$$

This standardised solubility expression was demonstrated to yield values for solubility of H, N and C in the Fe lattice with satisfactory accuracy [3]. In the case of analysis of C solubility in the Fe lattice, the factor B in Eq. (1) was taken to be 0. On the other hand, in the case of analysis of solubilities of H and N in the Fe lattice in the earlier work [3], $p(X_2)^{1/2}$ was used to represent $a(X)$.

In the present work, the $a(P)-T-C$ relationships determined experimentally for the molten $Fe_{1-y}Cr_yP_x$ in the analytical form (1) are analysed using statistical thermodynamics. The results obtained by the present analysis for the molten $Fe_{1-y}Cr_yP_x$ are compared with the earlier analysis results for molten FeP_x [4] obtained through analysis of solubility data reported by Ban-ya et al. [5, 6] from the equilibration experiment undertaken in P_2 gas for compatibility of the estimation results.

2. Analysis procedure and results

2.1. Data sets analysed

As reviewed in the preceding work [2], sets of values for the constants, A, B and C, in the solubility expression (1) were determined for y values, 0.061, 0.114, 0.180, 0.274, 0.376 and 0.465, alone. Other sets of data points containing less than 5 levels of T at a given combination of x and y were not included for the analysis. That is, only the data sets of x and y combinations for which $a(P)$ was specified for at least 8 levels of T were analysed to determine the expression of the normalised format (1) in the preceding preparatory work [2]. The determined values of coefficients, A, B and C, are listed in Table 1. The following statistical thermodynamic analysis is made considering that the numerical $a(P)-T-x$ relationships for given y are determined by Eq. (1) with the parameter values listed in Table 1. At each T for a given y, five sets of $a(P)$ vs. x relations were calculated by choosing an arbitrary value of $a(P)$ to make the

Table 1. Estimated values for the coefficients, A, B and C, in the solubility expression $x = A \cdot a(P) \cdot \exp(B \cdot \ln T + C/T)$ for molten $Fe_{1-y}Cr_yP_x$ reproduced from Ref. [2].

y	$A/10^4$	B	$C/10^4$
0.061	1.030	-1.392[*]	1.562
0.114	1.033	-1.411	1.666
0.180	1.031	-1.424	1.631
0.274	1.002	-1.406	1.594
0.375	1.028	-1.342	1.489
0.465	1.024	-1.223	1.269

[*] The parameter values were taken from Table 2 in Ref. [2] with a correction to the value for B at the composition $y = 0.061$ which was erroneously determined by a simple careless calculation mistake in converting the composition data given in atom fractions, $x(P) = 0.155$ and $x(Cr) = 0.054$, to erroneous $Fe_{0.939}Cr_{0.061}P_{0.130}$ instead of correct $Fe_{0.939}Cr_{0.061}P_{0.183}$.

Table 2. Values of $D(P_2)/2$, $[D(P_2)/2 – RT\,C(T)]$ and a factor $(0.0446T – 117.168)$ used for the present calculation.

T (K)	$D(P_2)/2^{<*>}$ (kJ · mol^{-1})	$D(P_2)/2 – RT\,C(T)^{<*>}$ (kJ · mol^{-1})	$0.0446T – 117.168^{<**>}$ (kJ · mol^{-1})
1400	247.659	411.920	−54.718
1500	247.873	425.824	−50.257
1600	248.090	439.855	−45.796
1700	248.304	453.998	−41.336
1800	248.525	468.259	−36.875

<*> $D(P_2)$ values were taken from *JANAF Thermochemical Tables* [16] and $[D(P_2)/2 – RT\,C(T)]$ was calculated according to Eq. (4).
<**> The factor $(0.0446T – 117.168)$ (kJ · mol^{-1}) corresponds to $(g – g')$ as expressed in Eq. (10).
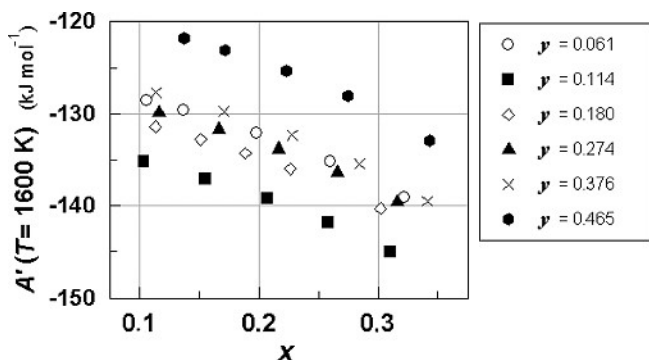

Fig. 1. $A'(T)$ vs. x isotherms at $T = 1600$ K calculated using Eq. (9) with the θ parameter value taken to be 0.50 by substituting with the numerical solubility data sets enumerated from Eq. (1) with the values of parameters, A, B and C, taken from Table 1.

composition x fall in the range between 0.10 and 0.35 with reference to the available equilibrium phase relationships for Fe–P and Cr–P systems [7–9].

For both Fe–P [7, 8] and Cr–P [7, 9] binary systems, the M_3P phase and the MP phase exist and in addition, near the di-metal phosphide composition (MP$_{0.50}$), Fe$_2$P for the Fe–P system and Cr$_{12}$P$_7$ for the Cr–P system are claimed to exist.

In the earlier statistical thermodynamic analysis for the molten Fe–P system [4], the value of the parameter θ representing the available number for occupation by the interstitial P atoms per Fe atom was chosen to be 0.50 to undertake valid analysis. When the θ value was taken to be 0.75 or 1.0, the derived isothermal A vs. x plots showed varying slope with x as exhibited in Fig. 1 in Ref. [4] implying varying $\beta E(P\text{-}P)$ with x. We judge that such variation of $E(P\text{-}P)$ with composition x in the homogeneity range of MP$_x$ simply signifies the inadequate selection of the statistical model because occurrence of such variation of interaction energy between interstitial atoms would lead to phase transformation rather than holding the same phase [4].

Taking into account this information together with the equilibrium phase relationships for Fe–P and Cr–P binary systems [7–9], the present numerical statistical thermodynamic calculation was carried out for the range of x smaller than 0.35 by choosing the parameter value θ to be equal to 0.50.

2.2. Statistical thermodynamic analysis

In the statistical thermodynamics, the partition function *PF* for a condensed phase (either solid or liquid) under consideration is composed taking into account the nearest neighbour atomic interactions. Then, from the partial derivation of *PF* with respect to the number n_i of a constituent element i in the condensed phase, chemical potential $\mu(i)^c$ of the constituent i in the condensed phase is derived. Then, $\mu(i)^c$ is put equal to $\mu(i)^g$ of the same element i in the gas phase.

The expression for $\mu(X)^g$ of an ideal diatomic gas X_2 is readily available in the classical text book authored by Fowler and Guggenheim [10]. The detailed derivation procedure of $\mu(X)^c$ for the condensed phase MX$_x$ can be referred to elsewhere [11–14]. Anyway, it is eventually reduced to the following set of equations for the purpose of analysing P solution in the present concern [4, 15]

$$A(T) \equiv RT \ln\{[p(P_2)]^{1/2} \cdot (\theta – x)/x\} = g + \beta x E(P\text{-}P) \quad (2)$$

$$K = g – [D(P_2)/2 – RT\,C(T)] = Q – RT \ln f_P(T) \quad (3)$$

$$C(T) = –(1/2) \ln \{[(4\pi m_P)^{3/2}\, k^{5/2}/h^3]$$
$$\times [(T^{7/2}/\Theta_r) \cdot (1 + \Theta_r/3T)] \cdot [\rho^2 v_0^*/2]\}$$
$$+ \Theta_v/4T + (1/2) \ln [1 – \exp(–\Theta_v/T)] \quad (4)$$

$$\ln f_P(T) = – \int_0^\infty g(v) \ln[1 – \exp(–hv/kT)]\, dv + \ln \rho v_0 \quad (5)$$

$$Q + \beta x E(P\text{-}P) = \partial E/\partial n_P \quad (6)$$

For starting the statistical thermodynamic analysis using Eq. (2), the value for the parameter θ must be chosen adequately to yield linear $A(T)$ vs. x isotherms. This is to fulfill the a priori assumption of constant $E(P\text{-}P)$ over a range of homogeneity composition x at a given T for Fe$_{1-y}$Cr$_y$P$_x$ of a given composition y. All the past statistical thermodynamic analyses for non-stoichiometric interstitial solution systems were made under this simplifying a priori assumption and the derived conclusions appeared to be realistic being compatible with the other available experimental evidence and so this assumption was considered to be valid although there is no first-principle-based justification to verify the validity of this a priori assumption [2–4, 11–15]. In the earlier analysis for the molten Fe–P system [4], the θ value was taken to be 0.50 as pointed out earlier in the text and so the following analysis is made with $\theta = 0.50$.

In addition, we need to modify the fundamental statistical thermodynamic formula Eq. (2) expressed as functions of $p(P_2)$, T and x, to an expression given as functions of $a(P)$, T and x. By so doing, we can use the present set of data

presented in form of $a(P)-T-x$ relationships for given y rather than in form of $p(P_2)-T-x$ relationships. For this conversion of the expression of the fundamental formula, the empirical $p(P_2)-a(P)$ conversion relationship presented by Ban-ya et al. [5] is used.

$$\log_{10}[p(P_2)^{1/2}/a(P)] = 2.33 - 6120/T \qquad (7)$$

As this formula was presented in engineering logarithm, it is converted to natural logarithm format to carry out the numerical calculation combined with the fundamental formula Eq. (2).

$$\ln[p(P_2)^{1/2}/a(P)] = 5.365 - 14092/T \qquad (8)$$

Then, the fundamental Eq. (2) is converted to the one as functions of $a(P)$, T and x in place of the one as functions of $p(P_2)$, T and x

$$A'(T) \equiv RT\ln[a(P)\cdot(\theta-x)/x] = g' + \beta x E(\text{P-P})$$

$$= [g - RT(5.365 - 14092/T)] + \beta x E(\text{P-P})$$

$$= (g + 117.168 - 0.0446T) + \beta x E(\text{P-P}) \qquad (9)$$

That is, desired values of g as a function of T to evaluate values of Q and $R\ln f_P$ using Eq. (3) can be determined from the intercept g' of A' vs. x plot at $x = 0$ by the relationship

$$g = g' + (0.0446T - 117.168) \ (\text{kJ}\cdot\text{mol}^{-1}) \qquad (10)$$

The calculation results for A' vs. x relationships at $T = 1600$ K are plotted in Fig. 1. As seen in Fig. 1, the derived $A'(T)$ vs. x isotherm with $\theta = 0.50$ at any examined composition y fell into a linear relationship to fulfill the a priori assumption of constant $E(\text{P-P})$ in the homogeneity composition range of the molten $\text{Fe}_{1-y}\text{Cr}_y\text{P}_x$. By undertaking similar calculations, the values of the parameters, $\beta E(\text{P-P})$ and g', in Eq. (9) for respective y values were determined as a function of T. These calculation results are presented in Fig. 2 ($\beta E(\text{P-P})$) and in Fig. 3 (g' values).

From the enumerated values of g', the values of g were calculated according to Eq. (10) and then the K vs. T plots exhibited in Fig. 4 were prepared using Eq. (3). Then, the values of Q and $R\ln f_P$ are estimated using values of $[D(P_2)/2 - RT\,C(T)]$ in Table 2. Calculation results are summarised in Table 3 together with the corresponding values of these parameters for molten FeP_x reported in the earlier work [4]. To visualise the calculation results, these values are plotted as shown in Fig. 5.

It is seen in Fig. 5 that Q in the molten $\text{Fe}_{1-y}\text{Cr}_y\text{P}_x$ showed the trend of increasing stability of P with the rising Cr content up to around 0.18 and then, with the further increase in P content, the stability of P in the molten $\text{Fe}_{1-y}\text{Cr}_y\text{P}_x$ tended to become less. The observed trend for variation of Q against y in Fig. 5 appears to correspond rationally with the observed rise of P solubility for molten $\text{Fe}_{1-y}\text{Cr}_y\text{P}_x$ with y increasing from 0 to 0.114 and the decrease in it with the further increase in y exceeding 0.18 (see Figs. 4 and 5 in Ref. [2]).

According to Zaitsev et al. [9], the congruent melting temperature of the Cr_{12}P_7 phase is 1723 °C while that of Fe_2P is 1370 °C and the temperature of Cr_3P melt to be in equilibrium with solid $\text{Cr}_{12}\text{P}7$ is 1506 °C while that of Fe_3P melt to be in equilibrium with solid Fe_2P is 1168 °C. This evidence appeared to suggest that the P–Cr bond is appreci-
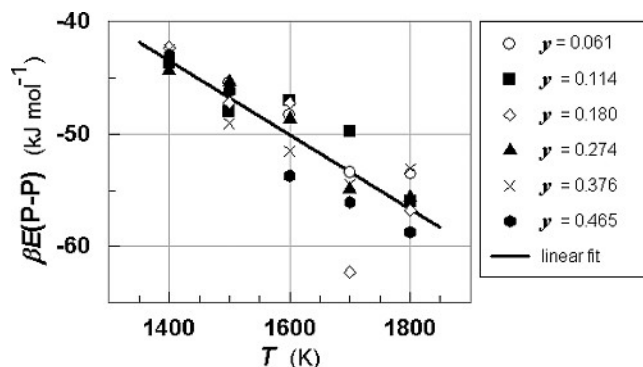
Fig. 2. Values of $\beta E(\text{P-P})$ estimated as the slope of $A'(T)$ vs. x isotherms with reference to Eq. (9).
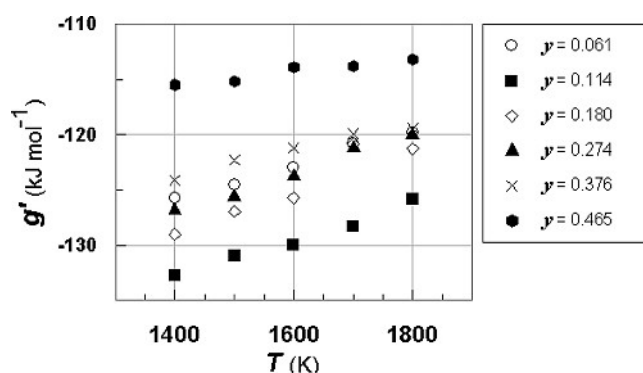

Fig. 3. Values of g' estimated as the intercept of $A'(T)$ vs. x isotherms at $x = 0$ with reference to Eq. (9).
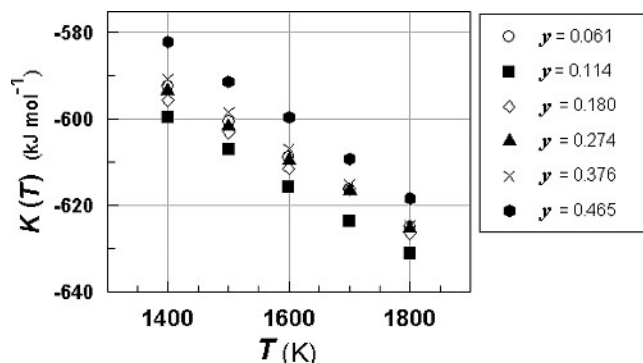

Fig. 4. Calculated $K(T)$ vs. T relationships for molten $\text{Fe}_{1-y}\text{Cr}_y\text{P}_x$.

Table 3. Estimated values for Q and $R\ln f_P$.

y	Q (kJ·mol^{-1})	$R\ln f_P$ (J·mol^{-1}·K^{-1})
0 (FeP$_x$)	−347.1	91.5
0.061	**−479.4**	80.7
0.114	**−487.7**	79.8
0.180	**−491.0**	74.7
0.274	**−483.8**	78.4
0.376	**−472.1**	84.4
0.465	**−455.7**	90.2

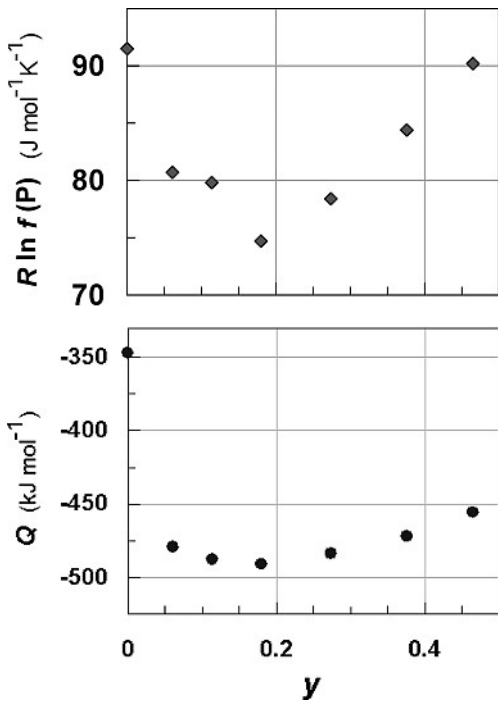<*> Values for Q and $R\ln f_P$ for FeP$_x$ ($y = 0$) are taken from Ref. [4] as the references.

Fig. 5. Estimated values for Q and $R \ln f_P$ for molten $Fe_{1-y}Cr_yP_x$.

ably tighter than the P–Fe bond and accordingly the observed significant drop in the Q value on the small proportion of alloying with Cr to Fe seen in Fig. 5 appears rational.

Detailed discussion for $R \ln f_P$ is not easy because of its rather complicated dependencies on several atomistic factors but the pattern of variation of it with respect to y appears to demonstrate some systematic change of electronic state around P in the molten $Fe_{1-y}Cr_yP_x$ with Cr content y.

Similar systematic variations of Q and $R \ln f_X$ with respect to the composition y of two metallic constituents $(M_I)_{1-y}(M_{II})_yX_x$ were also observed for C solubility in fcc (face centred cubic) $Fe_{1-y}Co_y$ and $Co_{1-y}Ni_y$ alloy lattices showing smooth transition along the alloy composition across the groups in the Periodic Table of the Elements, Fe through Co to Ni, as exhibited in Fig. 2 in Ref. [17].

This evidence appears to support indirectly the validity of the present statistical thermodynamic analysis as well as the validity of the empirical solubility expression derived in the preceding publication [2].

3. Interpolating estimation of a(P) for given combination of x and y at arbitrary T

As reviewed above, the present estimation results looked generally reasonable. Thus, the feasibility of reproducing the experimental data from the estimated set of statistical thermodynamic parameters is examined briefly in the following.

For this, g' and βE(P-P) determined for given y on the basis of Eq. (9) are used. That is, we start from

$$RT \ln[a(\text{P}) \cdot (0.50 - x)/x] = g' + \beta x E(\text{P-P}) \qquad (11)$$

By re-writing this equation, we obtain

$$a(\text{P}) = [x/(0.50 - x)] \cdot \exp\{[g' + \beta x E(\text{P-P})]/RT\} \qquad (12)$$

We undertake the following interpolating estimation using this equation for the data sets, group III containing the test runs Nos. 17～20 and group XV containing the test runs Nos. 80～84 (see Table 4) [1, 2].

As plotted in Fig. 2, βE(P-P) values for given y varied with T showing some scatter. To simplify the estimation, we assume that the variation of βE(P-P) is roughly represented as a function of T alone

$$\beta E(\text{P-P}) = 2.656 - 0.033T \; (\text{kJ} \cdot \text{mol}^{-1}) \qquad (13)$$

This equation was determined by simple least-mean-squares fitting of all the data points in Fig. 2.

On the other hand, expressions for g' used for the present estimation are

$$g'(y = 0.180) = -159.228 + 0.0215T \; (\text{kJ} \cdot \text{mol}^{-1}) \qquad (14)$$

$$g'(y = 0.114) = -155.916 + 0.0165T \; (\text{kJ} \cdot \text{mol}^{-1}) \qquad (15)$$

The g' values for $y = 0.159$ and $y = 0.130$ are determined by interpolating the constant term and the factor for T independently

$$g'(y = 0.159) = -158.174 + 0.0199T \; (\text{kJ} \cdot \text{mol}^{-1}) \qquad (16)$$

$$g'(y = 0.130) = -156.719 + 0.0177T \; (\text{kJ} \cdot \text{mol}^{-1}) \qquad (17)$$

The calculated a(P) values listed in Table 4 were obtained using Eq. (12) by substituting βE(P-P) with Eq. (13) and g' with either Eq. (16) or (17).

As seen in Table 4, the calculated values for a(P) for group III data ($y = 0.159$ and $x = 0.050$) were about double that of the experimental values while those for group XV ($y = 0.130$ and $x = 0.325$) were about 4-fold

Table 4. Interpolating estimation of a(P) for molten $Fe_{1-y}Cr_yP_x$ for given combinations of y and x at arbitrary temperature T.

Group #	Run #	$Fe_{1-y}Cr_yP_x$	T (K)	a(P)	
				experimental	calculated
III	17	$Fe_{0.841}Cr_{0.159}P_{0.050}$	1728	0.000008	0.000017
	18		1759	0.000009	0.000020
	19		1787	0.000011	0.000024
	20		1811	0.000012	0.000028
XV	80	$Fe_{0.870}Cr_{0.130}P_{0.325}$	1561	0.000119	0.000026
	81		1603	0.000155	0.000036
	82		1654	0.000204	0.000051
	83		1708	0.000276	0.000073
	84		1812	0.000472	0.000138

smaller than the experimental values. These extents of deviations of the calculated $a(P)$ from the corresponding experimental data might be due to the crudeness of the present estimation using coarse approximation for $\beta E(\text{P-P})$ as practiced above using simplifying Eq. (13) while it actually depends on y as well as on T. It is easily noticed in Fig. 2 that $\beta E(\text{P-P})$ for different y tended to deviate more widely from the simplifying linear relationship when T increased. Anyway, in spite of the crudeness of the approximation, the order of magnitude of the estimated $a(P)$ was comparable to that of the corresponding experimental data. Thus, the statistical thermodynamic parameter obtained for the molten $Fe_{1-y}Cr_yP_x$ at different y values might be used to estimate the $a(P)-T-x$ relationship for arbitrary y level by interpolation to get a rough idea about the correlation between $a(P)$ and x for given y at arbitrary T for molten $Fe_{1-y}Cr_yP_x$.

In the above brief test, the calculation was made based on g' using Eq. (9) instead of being based on g using Eq. (2). This might be another possible cause leading to the appreciable deviation of the calculated $a(P)$ from the experimental $a(P)$ and the margin of error might be diminished by estimation using g in place of g'.

4. Concluding remark

The analytical $a(P)-T-x$ relationships evaluated for a number of y values for molten $Fe_{1-y}Cr_yP_x$ in the recent work [2] from the discrete set of $a(P)-T-x$ data reported by Zaitsev et al. [1] were analysed by statistical thermodynamics.

The results of the statistical thermodynamic analysis appear to be acceptable exhibiting a realistic pattern of variation of the Q parameter with y showing rational correspondence with the observed variation pattern of P solubility in molten $Fe_{1-y}Cr_yP_x$ although no special tendency of cluster formation by Fe and Cr atoms around the P atom was concluded. Up to $y = 0.18$ in molten $Fe_{1-y}Cr_yP_x$, the extent of the stabilisation of P atoms in the molten lattice seemed to become higher with increasing y but then, in the range of y higher than 0.18, the extent of the stabilisation of P atoms in the molten lattice seemed to become less with increasing y.

It was also demonstrated that the $a(P)-x$ relationship for arbitrary composition y at specified temperature T might be estimated with acceptable precision by interpolating simulation using the estimated values of $\beta E(\text{P-P})$ and g' for two known levels of y.

APPENDIX/List of symbols

$a(P)$: chemical activity of P atom

$A(T)$: $\equiv RT \ln\{[p(P_2)]^{1/2} \cdot (\theta - x)/x\}$ (kJ · mol^{-1}); calculated from experimentally determined values of $p(P_2)$, T and x for specified value of θ using Eq. (2)

$A'(T)$: $\equiv RT \ln [a(P) \cdot (\theta - x)/x]$ (kJ · mol^{-1}); calculated from experimentally determined values of $a(P)$, T and x for specified value of θ using Eq. (9)

A, B and C: proportionality constants in Eq. (1)

$C(T)$: defined by Eq. (4) to represent contributions of translational, rotational and vibrational motions of P_2 molecule

$D(P_2)$: dissociation energy of P_2 molecule per mole (kJ · mol^{-1})

E: lattice energy (kJ · mol^{-1})

$E(i-j)$: nearest neighbour pair-wise interaction energy between i and j atoms in molten $Fe_{1-y}Cr_yP_x$ lattice

$f_P(T)$: partition function of P atom in molten $Fe_{1-y}Cr_yP_x$ lattice at T

g: parameter determined as the intercept of the $A(T)$ vs. x plot at $x = 0$ using Eq. (2)

g': parameter determined as the intercept of the $A'(T)$ vs. x plot at $x = 0$ using Eq. (9)

$g(\nu)$: distribution function

h: Planck constant

k: Boltzmann constant

K: parameter calculated from g using Eq. (3)

m_P: mass of P atom

n_P: number of P atoms in molten $Fe_{1-y}Cr_yP_x$ lattice

$p(P_2)$: partial pressure of ideal P_2 gas molecule (bar)

$P-T-C$: pressure–temperature–composition

Q: degree of stabilisation of P atom in molten $Fe_{1-y}Cr_yP_x$ lattice with reference to isolated P atom in vacuum

R: universal gas constant (= 0.0083145 kJ · mol^{-1})

T: absolute temperature (K)

x: atom fraction of P against total metal in molten $Fe_{1-y}Cr_yP_x$

y: atom fraction of Cr in the metal lattice in molten $Fe_{1-y}Cr_yP_x$

β: factor determined from crystal structure consideration

θ: number of available interstitial sites for occupation by P atom per metal atom in $Fe_{1-y}Cr_y$ lattice

Θ_r: characteristic temperature for rotation of P_2 molecule (= 0.436 K) <*1>

Θ_v: characteristic temperature for vibration of P_2 molecule (= 1123 K) <*2>

$\mu(X)^c$: chemical potential of X atom in the condensed phase MX_x

$\mu(X)^g$: chemical potential of X atom in the ideal diatomic X_2 gas molecule

ν: vibrational frequency of P atom in molten $Fe_{1-y}Cr_yP_x$ lattice

ρ: nuclear spin weight (taken to be 1)

υ_0: statistical weight of tightly bound electrons around P in molten $Fe_{1-y}Cr_yP_x$ lattice

υ_0^*: electronic state of P_2 molecule in normal state (taken to be 1)

<*1> This value of $\Theta_r(P_2) = 0.436$ K was calculated from $B_e = 0.30327$ cm^{-1} listed for ideal diatomic gas P_2 in JANAF Thermochemical Tables [16] using a conversion factor 1 cm^{-1} = 1.4388 K.

<*2> This value of $\Theta_v(P_2) = 1123$ K was calculated from $\omega_e = 780.43$ cm^{-1} [16].

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